Critical properties of the half-filled Hubbard model in three dimensions

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By means of the dynamical vertex approximation (DΓA) we include spatial correlations on all length scales beyond the dynamical mean field theory (DMFT) for the half-filled Hubbard model in three dimensions. The most relevant changes due to non-local fluctuations are: (i) a deviation from the mean-field critical behavior with the same critical exponents as for the three dimensional Heisenberg (anti)-ferromagnet and (ii) a sizable reduction of the Néel temperature (T_N) by $\sim 30\%$ for the onset of antiferromagnetic order. Finally, we give a quantitative estimate of the deviation of the spectra between DΓA and DMFT in different regions of the phase-diagram.

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Almost 50 years after the invention of the Hubbard model [1] and despite modern petaflop supercomputers, a precise analysis of the criticality of this most basic model for electronic correlations has not been achieved so far, at least not in three dimensions. Dynamical mean field theory (DMFT) [2–4] was a big step forward to calculate the three dimensional Hubbard model since the major contribution of electronic correlations, i.e, the local one, is well captured within this theory. Local correlations give rise to quasiparticle renormalization, the Mott-Hubbard transition, magnetism, and even more subtle issues such as kinks in purely electronic models [5]. However, non-local spatial correlations are also naturally generated by a purely local Hubbard interaction, and, as it is well known, they become of essential importance in the vicinity of second-order phase transitions. As these correlations are neglected in DMFT, this scheme provides only for a conventional mean-field (MF) description of the critical properties.

To overcome this shortcoming cluster extensions to DMFT such as the dynamical cluster approximation (DCA) and cluster-DMFT have been proposed [6]. In these approaches spatial correlations beyond DMFT are taken into account, however only within the range of the cluster size; and due to computational limitations the actual size of $d = 3$-clusters is restricted to about 100 sites. Hence, short-range correlations are included by these approaches, whereas long-range ones are not (e.g. for spacings larger than 5 lattice sites in $d = 3$). Nonetheless, Kent *et al.* [7] were able to extrapolate the cluster size of so-called Betts clusters to infinity, albeit assuming from the beginning the critical exponents to be those of the Heisenberg model. This way they extrapolated the Néel temperature of the paramagnetic-to-antiferromagnetic phase transition which was found in agreement with earlier lattice quantum Monte Carlo (QMC) results by Staudt *et al.* [8].

As an alternative to cluster extensions and, in particular, to include long-range correlations on an equal footing, more recently diagrammatic expansions of DMFT have been proposed: (i) the DMFT plus spin-fermion model [9], (ii) the dynamical vertex approximation (DΓA) [10–12] which approximates the fully irreducible n-particle vertex to be local [10] or that of a DCA cluster [12]; and (iii) the dual fermion approach [13]. As for phase transitions, DΓA with Moriyasque corrections [14] fulfills - in contrast with dual fermion calculations of [15]- the Mermin and Wagner theorem in two-dimensions and, as we will discuss in the following, corrects the MF behavior for the critical exponents in three dimensions.

In this paper, we apply the aforementioned approximation of the DΓA scheme (with Moriyasque corrections [14]) for studying the phase-diagram of the three dimensional Hubbard model at half-filling. In particular, we (i) calculate the critical exponents, (ii) determine the phase diagram with T_N substantially reduced compared to the DMFT one, and (iii) define the region where non-local correlations become too strong so that DMFT is not applicable anymore.

We consider the Hubbard model on a cubic lattice

$$H = -t \sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

where t denotes the hopping amplitude between nearest-neighbors, U the Coulomb interaction, and $c^\dagger_{i\sigma}(c_{i\sigma})$ creates (annihilates) an electron with spin σ on site i; $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. In the following, we restrict ourselves to the paramagnetic phase with $n = 1$ electron/site at a finite temperature T. For the sake of clarity, and in accordance with previous publications, we will define hereafter our energies in terms of a typical energy scale $D = 2\sqrt{6}\,t$ [16].

The DΓA approach to the model (1) was derived in Refs. 10 and 14. The dynamic non-uniform susceptibility reads

$$\chi^{s(c)}_{\mathbf{q}\omega} = [(\phi^{s(c)}_{\mathbf{q},\omega})^{-1} \mp U + \lambda_{s(c)}]^{-1} \qquad (2)$$

with $\phi^{s(c)}_{\mathbf{q},\omega} = \sum_{\nu\nu'} \Phi^{\nu\nu'\omega}_{s(c),\mathbf{q}} = \sum_{\nu\nu'} [(\chi^{\nu'}_{0\mathbf{q}\omega})^{-1}\delta^{\nu'}_{\nu} - \Gamma^{\nu\nu'\omega}_{s(c)\mathrm{ir}} \pm U]^{-1}$, $\chi^{\nu'}_{0\mathbf{q}\omega} = -T\sum_{\mathbf{k}} G_{\mathbf{k},\nu'} G_{\mathbf{k}+\mathbf{q},\nu'+\omega}$ (particle-hole bub-

ble), $G_{\mathbf{k},\nu} = [i\nu - \epsilon_{\mathbf{k}} + \mu - \Sigma_{\rm loc}(\nu)]^{-1}$ (Green function) and $\Sigma_{\rm loc}(\nu)$ (local self-energy). The vertex $\Gamma^{\nu\nu'\omega}_{s(c),\rm ir}$ is determined from the solution of the single-impurity problem[10]. In fact, the complete inclusion of non-local corrections in the irreducible vertices in all channels can be achieved only via the fully self-consistent DΓA equations. However, as discussed in Ref. [14], when considering a situation where no competition between different instabilities occurs, a restriction to one specific channel and the evaluation of the self-consistency effect via the corresponding Moriyasque correction $\lambda_{s(c)}$ is possible [14]. In the half-filled case we neglect non-local particle-particle fluctuations since this channel is strongly suppressed by the repulsive interaction. Furthermore, at half filling, charge excitations are generically expected to be irrelevant for the critical behavior as well. Indeed we find $\chi^{c}_{\mathbf{q}\omega}, \chi^{pp}_{\mathbf{q}\omega} \ll \chi^{s}_{\mathbf{q}\omega}$ ($\chi^{pp}_{\mathbf{q}\omega}$ is the particle-particle susceptibility), hence we neglect non-local particle-particle contributions as well as λ_c and determine λ_s from the exact sum rule (which also holds for DMFT) $-\int_{-\infty}^{\infty}\frac{d\nu}{\pi}{\rm Im}\Sigma_{\mathbf{k},\nu} = U^2 n(1-n/2)/2$, where the non-local self-energy is given by

$$\Sigma_{\mathbf{k},\nu} = \frac{1}{2}Un + \frac{1}{2}TU\sum_{\omega,\mathbf{q}}\Big[3\gamma^{\nu\omega}_{s,\mathbf{q}} - \gamma^{\nu\omega}_{c,\mathbf{q}} - 2 + 3U\gamma^{\nu\omega}_{s,\mathbf{q}}\chi^{s}_{\mathbf{q}\omega} + U\gamma^{\nu\omega}_{c,\mathbf{q}}\chi^{c}_{\mathbf{q}\omega} + \sum_{\nu'}\chi^{\nu'}_{0\mathbf{q}\omega}(\Gamma^{\nu\nu'\omega}_{c,\rm loc} - \Gamma^{\nu\nu'\omega}_{s,\rm loc})\Big]G_{\mathbf{k}+\mathbf{q},\nu+\omega} \quad (3)$$

with $\gamma^{\nu\omega}_{s(c),\mathbf{q}} = (\chi^{\nu}_{0\mathbf{q}\omega})^{-1}\sum_{\nu'}\Phi^{\nu\nu'\omega}_{s(c),\mathbf{q}}$, and $\Gamma^{\nu\nu'\omega}_{s(c),\rm loc}$ is the reducible local spin (charge) vertex, determined from the single-impurity problem.

Starting point of our investigation of the critical properties of the antiferromagnetic (AF) instability is the corresponding (divergent) spin susceptibility

$$\chi_{AF} = \chi^{s}_{\mathbf{Q},0} = \int_0^{\beta} d\tau \langle S_{z,\mathbf{Q}}(\tau) S_{z,-\mathbf{Q}}(0)\rangle \quad (4)$$

with $\mathbf{Q} = (\pi,\pi,\pi)$. While the DΓA with Moriyasque corrections well reproduces the textbook Mermin and Wagner results for the Hubbard model in $d=2$ yielding finite, but exponentially large susceptibility at finite T [14], the situation in $d=3$ is even more intriguing, since the AF-phase remains stable in a broad region at finite T, allowing for a direct study of the critical properties.

Of particular interest is the analysis of the evolution of the critical region as a function of the Coulomb repulsion. In Fig. 1, we show the inverse susceptibility χ^{-1}_{AF} as a function of T for different U values. The vanishing of $\chi^{-1}_{AF} \propto (T-T_N)^{\gamma}$ marks the onset of the AF long-range order, defining the corresponding T_N for a given U. More important is, however, the examination of the critical behavior: While in a MF (or DMFT) approach χ^{-1}_{AF} is vanishing linearly close to T_N in accordance with the MF (Gaussian) critical exponent $\gamma = 1$ (see lower inset

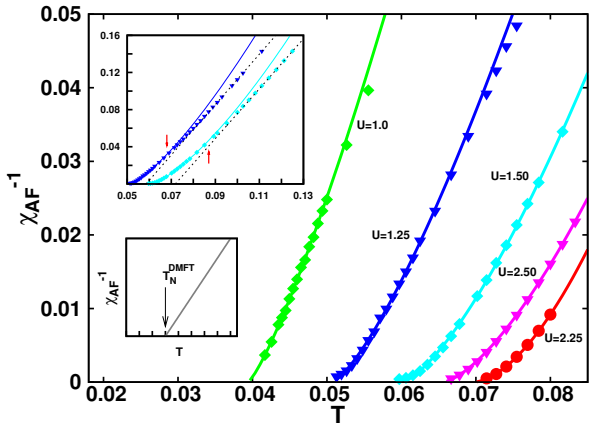

FIG. 1. (Color online) Inverse AF spin susceptibility as a function of T for different U values. Lower inset: Inverse DMFT susceptibility with a MF ($\gamma = 1$: linear behavior) critical exponent. Upper inset: larger T interval.

of Fig. 1), DΓA data clearly show a bending in the region close to the AF transition (i.e., for $T < T_G$, the so-called Ginzburg temperature), indicating a DΓA critical exponent γ definitely larger than 1. The non-perturbative nature of DΓA also allows for a treatment of the critical behavior, e.g. the size of the critical region, as a function of U: From our data it emerges that, in the U-range studied, the size of the region where the critical behavior deviates from the MF predictions (here: from linearity) increases with U. In order to quantify this statement, we have performed DΓA calculations at higher T (upper inset of Fig.1) for U up to 1.5, and fitted the data linearly in the high-T regime. T_G has been hence estimated as the temperature below which the relative deviation of χ^{-1}_{AF} from the above-mentioned linear fit becomes larger than 10% (red arrows in the upper inset of Fig. 1). By this criterion for T_G, the size of the critical region with non-MF behavior, i.e. $\Delta T_{crit} = T_G - T_N$, increases from $\simeq 0.01$ for $U=1.0$, to $\simeq 0.02$ for $U=1.25$ and $\simeq 0.025$ for $U=1.5$, following therefore the dependence determined by the Ginzburg criterion, which implies the inapplicability of the standard Landau-Ginzburg expansion in the temperature region $\Delta T_{crit} \propto T_N^2$ [17]. For $U < 1$ (not shown) the bending of χ^{-1}_{AF} becomes hardly visible, since in this regime $T_N \sim {\rm e}^{-\frac{1}{WU}}$ (with $W \propto 1/D$), and therefore the size of the critical region is rather narrow; the linear behavior for $U > 1.5$ becomes confined to temperatures even higher than those shown in Fig. 1.

A more quantitative study of the critical behavior requires also a precise evaluation of the critical exponent(s). From the behavior of the spin-susceptibility, one can extract the values of the critical exponent ν, which controls the divergence of the AF-correlation length ξ (defined as the square root of the inverse mass of the spin-spin propagator at $\mathbf{q} = \mathbf{Q}$, $\omega = 0$) when $T \to T_N$. This can be computed either from the divergence of χ_{AF} (i.e., di-

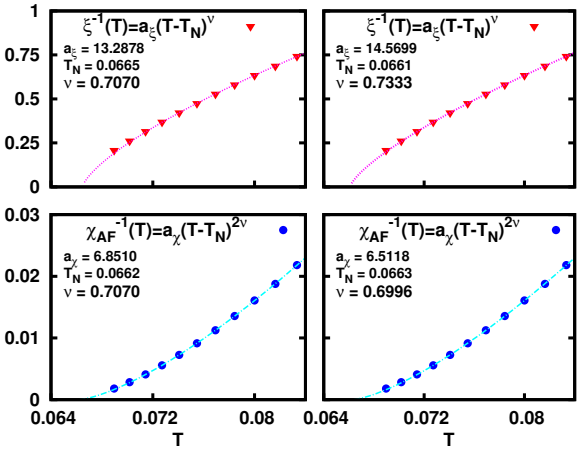

FIG. 2. (Color online) Fit of $\chi_{AF}^{-1}(T)$ and ξ^{-1}(T) for the highest interaction value considered, i.e., $U = 2.5$. Left: fit with fixed $\nu = 0.707$ (Heisenberg-exponent in $d = 3$ [20]). Right: free fit, showing the good compatibility with the $d=3$ Heisenberg universality class.

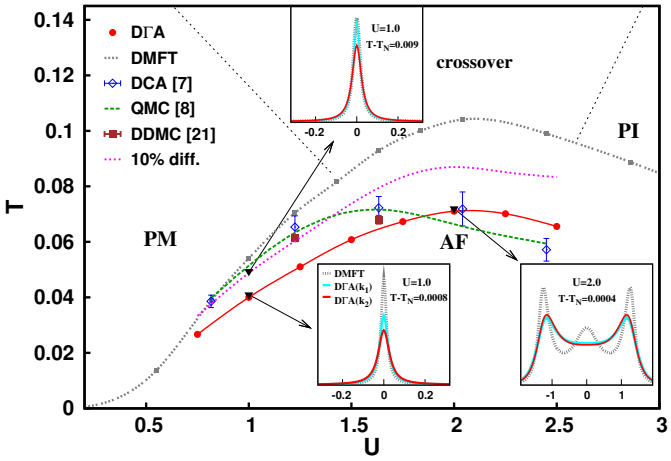

FIG. 3. (Color online) Néel Temperature in DΓA, compared with the corresponding DMFT, DCA, QMC and DDMC ones. Also shown is the region where corrections to DMFT in form of non-local correlations become dominant (violet dashed-dotted line: 10 % relative change between the DMFT and the DΓA self-energies at the lowest Matsubara frequency). Inset: DMFT vs. DΓA spectral functions (see text).

rectly from the data shown in Fig. 1), using the relation $\gamma = 2\nu$ [18], or by extracting from χ_{AF} the value of ξ by fitting its **q**-dependence for different T [19].

The results of our analysis, shown in Fig. 2, demonstrate that DΓA can describe well the AF criticality of the Hubbard model. For the largest values of $U = 2.5$, indeed, both divergences of χ_{AF} and ξ observed in DΓA can be described (left panels of Fig. 2) with high-accuracy by the critical exponent $\nu = 0.707$ of the $d = 3$-Heisenberg AF. This is expected to be the correct exponent, not only because the half-filled Hubbard can be mapped onto the Heisenberg model but also since dimension and symmetry of the order parameter suggest the same universality class. Similar results, though with a lower degree of precision, can be found by directly fitting the value of the ν exponent to χ_{AF}^{-1} and ξ (right panels): For $U = 2.5$, our two fits provide an estimate of $\nu \sim 0.70$ and 0.73, respectively. This shows the Heisenberg universality is still valid also in a parameter region (i.e., at intermediate coupling), where the Hubbard model is not well approximated by the Heisenberg model [21].

A natural by-product of the calculations of the critical exponents is the determination of T_N at the DΓA level, whose values overall well agree with the most accurate DCA and QMC/DDMC data (see Fig. 3). The deviations around $U = 1$ might originate from neglecting the rather small non-local corrections of the charge- and particle-particle-channels, which could affect non-universal quantities such as T_N. On the other hand, also the DCA/QMC finite-size extrapolation is difficult in this region since the AF correlation length is large. Let us also note that in this regime the DΓA self-energy compares well with the DCA one of Ref. [23] ($U = 1.633, T = 0.0714$): The deviation $\frac{1}{N}\sum_n |\mathrm{Im}\,\Sigma_{D\Gamma A}(\mathbf{k},\omega_n) - \mathrm{Im}\,\Sigma_{DCA}(\mathbf{k},\omega_n)|/|\mathrm{Im}\,\Sigma_{D\Gamma A}(\mathbf{k},\omega_n)|$ is $< 5\%$ in the sum over the first $N = 7$ Matsubara frequencies (i.e, for those, where a deviation from DMFT is observable). This is within the DCA difference between the two largest clusters considered (84 and 100 sites).

Finally, we investigate the effects of the non-local corrections on the spectral properties of the $d = 3$ Hubbard model. On general grounds, the maximum impact of non-local corrections is to be expected close to the second-order transition line. This is because the corresponding spin susceptibility, which explicitly enters in the DΓA equations for Σ, is diverging at the transition (red line in Fig. 3). Such behavior is particularly evident in the spectra shown in the two lower insets of Fig. 3 for temperatures slightly above the T_N of DΓA. Specifically, we compared paramagnetic DMFT and DΓA spectral functions at two different **k**-points on the Fermi Surface (FS) [24], i.e. $k_1 = (\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2})$, $k_2 = (\pi, 0, \frac{\pi}{2})$. At weak-coupling ($U = 1$) we observe a strong broadening of the DMFT quasiparticle (QP) peak. At $U = 2$, the enhanced scattering by non-local spin fluctuations even qualitatively changes the spectra: the (already) damped QP peak of DMFT is transformed into a "pseudogap" in DΓA. In principle, one can expect pseudogap behavior very close to the Néel temperature also for an arbitrarily small Coulomb interaction. The corresponding region appears, however, at small U very narrow: a qualitative estimate according to equ. (3) yields the condition for the pseudogap behavior $\xi > 4\pi v_F^3/(T_N U^2)$ (v_F is an average Fermi velocity), which can be hardly fulfilled at small U, where T_N is exponentially small. Outside the pseudogap region, AF fluctuations yield only an increase of the scattering rate $\gamma(\mathbf{k}) = -\mathrm{Im}\,\Sigma(\mathbf{k}, \omega = 0)$: e.g., at $T \sim T_N$ and

$U = 1$ we obtain $\gamma_{DMFT} = 0.02$, $\gamma_{D\Gamma A}(k_1) = 0.033$, and $\gamma_{D\Gamma A}(k_2) = 0.041$.

By increasing T, non-local corrections become naturally weaker, since AF-fluctuations are reduced in intensity and spatial extension, see, e.g., the temperature behavior of ξ in Fig. 2. As a criterion to evaluate the impact of non-local correlations, valid for the "pseudogap" as well as for insulating spectra, we have chosen the relative change between the DΓA and DMFT self-energy at the lowest Matsubara frequency: $|\Sigma_{\rm DMFT}(i\nu_1) - \Sigma_{\rm DGA}(\mathbf{k}_2, i\nu_1)|/|\Sigma_{\rm DMFT}(i\nu_1)|$. Note that this criterion is directly related to the QP weight Z in the metallic phase if the linear low frequency behavior of the self-energy already holds (approximately) at the lowest Matsubara frequency $i\nu_1$. By this one-particle criterion, DMFT is reliable down to the violet line in Fig. 3 below which deviations exceed 10%. Above this line, the impact of the non-local correlations on the spectral functions appears indeed moderate (upper inset of Fig. 3): this is also confirmed by the analysis of the spectral function, where the QP weight Z is unchanged (within errors) from the DMFT value ($Z = 0.76$) and the enhancement of γ is much smaller than before ($\gamma_{DMFT} = 0.027$, $\gamma_{D\Gamma A}(k_1) = 0.028$, $\gamma_{D\Gamma A}(k_2) = 0.036$).

While our findings may validate (a posteriori) the usage of DMFT for computing spectral functions in $d=3$, provided one is not interested in the immediate vicinity of (second-order) magnetic instabilities, it is important to note that the width of the critical region is not small at intermediate U. For instance, we observe that the size of the critical region ΔT_{crit} at $U > 1.25$ exceeds the violet line. Significant effects of non-local correlations may occur even further away from the AF-transition, depending on the quantity under consideration. In particular relevant deviations from the DMFT predictions at even higher-Ts have been reported when analyzing the temperature dependence of the entropy [22].

In conclusion, we have analyzed non-perturbatively the effect of non-local correlations in the $d = 3$ half-filled Hubbard model by means of DΓA. When considering regions where spatial correlations strongly modify the DMFT physics, which is particularly true close to magnetic instabilities, DΓA represents a very powerful tool for studying the critical properties beyond the MF/DMFT level: critical exponents of the Hubbard model are found to be -within the error bars- identical to those of the $d = 3$ Heisenberg model, and DΓA provides also for a proper reduction of T_N w.r.t. the DMFT prediction. Moreover, since the DΓA scheme includes both spatial and temporal electronic correlations in a non-perturbative way, it looks naturally very promising also for future analysis of quantum phase transitions beyond the weak-coupling regime.

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[1] J. Hubbard, Proc. Roy. Soc. London A **276** 238 (1963); M. C. Gutzwiller, Phys. Rev. Lett. **10** 159 (1963); J. Kanamori, Progr. Theor. Phy. **30**, 275 (1963).
[2] W.Metzner and D.Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[3] A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992).
[4] A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
[5] K. Byczuk, *et al.*, Nature Physics **3**, 168 (2007); A. Toschi, *et al.* Phys. Rev. Lett., **102**, 076402 (2009).
[6] T. Maier *et al.*, Rev. Mod. Phys. **77** 1027 (2005); G. Kotliar *et al.*, Phys. Rev. Lett. **87** 186401 (2001); A. I. Lichtenstein and M. I. Katsnelson, Phys. Rev. B **62** 9283 (R) (2000).
[7] P. R. C. Kent *et al.*, Phys. Rev. B **72**, 060411 (2005).
[8] R. Staudt, M. Dzierzawa, and A. Muramatsu, Eur. Phys. J. B **17**, 411 (2000).
[9] E. Z. Kuchinskii, I. A. Nekrasov and M. V. Sadovskii, Sov. Phys. JETP Lett. **82** 98 (2005).
[10] A. Toschi, A. A. Katanin, and K. Held. Phys. Rev. B **75**, 045118 (2007); Prog. Theor. Phys. Supp. **176**, 117 (2008).
[11] H. Kusunose, J. Phys. Soc. Jpn. **75**, 054713 (2006).
[12] C. Slezak *et al.* J. Phys.: Condens. Matter **21**, 435604 (2009).
[13] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B **77**, 033101 (2008).
[14] A. A. Katanin, A. Toschi, and K. Held, Phys. Rev. B **80**, 075104 (2009).
[15] S. Brener *et al.*, Phys. Rev. B **77**, 195105 (2008).
[16] With this choice, for $D = 1$, the standard deviation of our $d = 3$-DOS is equal to 0.5 as in several previous DMFT and DΓA calculations.
[17] L. D. Landau and E. Lifschitz, "Statistical Physics", volume V, p. 476, Eq. (146.15), Pergamon Press (1980).
[18] Note that within Moriyasque DΓA, the index η is not changed from its MF value (i.e., 0), since the explicitly **q**-dependent terms of the spin-spin propagator (but not its mass!) is computed at the level of DMFT.
[19] The value of ξ has been computed by fitting the DΓA spin susceptibility $\chi(\mathbf{q}, \Omega = 0)$ with the fitting function $\chi_{fit} = A/[4(\sin^2(\frac{q_x-\pi}{2})+\sin^2(\frac{q_y-\pi}{2})+\sin^2(\frac{q_z-\pi}{2}))+\xi^{-2}]$.
[20] M.F. Collins, "Magnetic Critical Scattering", Oxford University Press, New York, 1989.
[21] Note: For the Mott-Hubbard transition in paramagnetic Cr-doped V_2O_3 deviations from MF critical exponents have been found only in a tiny parameter region , see P. Limelette *et al.*, Science **302**, 89 (2003).
[22] S. Fuchs et al., Phys. Rev. Lett. **106**, 030401 (2011).
[23] E. Gull *et al.*, Phys. Rev. B **83**, 075122 (2011).
[24] This choice is highly significant, because for these **k**-points (at the FS) the largest/smallest deviations from the DMFT self-energy are found.
[25] E. Gull *et al.*, Phys. Rev. B **82**, 155101 (2010).